

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 339 °C

Global applicability domain: Outside

Local applicability domain index: 1.71e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

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Measured: 345

Predicted: 341

Image not found

Ametryn

Measured: 345

Predicted: 341

Image not found

2,4,6-Tricyano-1,3,5-triazine

Measured: 262

Predicted: 264

Image not found

3-Methyl-1-phenyl-1H-pyrazol-5-amine

Measured: 333

Predicted: 334

Image not found

4-Aminoazobenzene

Measured: 366

Predicted: 337